

Precision analysis of Geant4 condensed transport effects on energy deposition in detectors

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Abstract. A comprehensive analysis of the effects of Geant4 algorithms for condensed transport in detectors is in progress. The first phase of the project focuses on electron multiple scattering, and studies two related observables: the longitudinal pattern of energy deposition in various materials, and the fraction of backscattered particles. The quality of the simulation is evaluated through comparison with high precision experimental measurements; several versions of Geant4 are analyzed to provide an extensive overview of the evolution of Geant4 multiple scattering algorithms and of their contribution to simulation accuracy.

1. Introduction

Physics models and computational algorithms operating in the condensed transport scheme - multiple scattering and energy loss of charged particles - play a critical role in the simulation of energy deposition in detectors. Previous studies [1, 2] have highlighted the contribution of Geant4 [3, 4] multiple scattering implementation to simulate the longitudinal profile of the energy deposited by electrons and protons in matter, and its effects on the accuracy of the simulation with respect to experimental measurements. Nevertheless, despite the relevance of Geant4 condensed transport to experimental applications, a comprehensive overview of the problem domain is still missing: quantitative comparisons with experiment for model validation are relatively scarce in the literature, and the interplay of algorithms and model parameters on different observables has not been quantified yet.

A project in progress analyzes the effects of algorithms for condensed transport of electrons in Geant4, namely of multiple scattering. It evaluates the contribution to simulation accuracy of a variety of Geant4 multiple scattering models with respect to high precision experimental measurements of the longitudinal pattern of energy deposition, and of the fraction of backscattered particles.

Geant4 multiple scattering simulation involves a number of parameters and physics modeling approaches, which have been subject to modifications in the course of the years. The results reported in the above mentioned references show significant variations in the simulation outcome depending on Geant4 versions, which reflect the ongoing evolution of Geant4. Due to the fast pace of new Geant4 version releases and correction patches, several Geant4 versions are concurrently in use in the experimental community; therefore, the validation analysis of the effects of multiple scattering implementations is extended to a number of recent Geant4 versions.

This paper reflects the limited amount of information that could be presented in a poster at the CHEP (Computing in High Energy Physics) 2012 conference; the full set of results will be extensively documented in a dedicated journal publication.

2. Overview of Geant4 multiple scattering models

Geant4 original multiple scattering model [5], also known as the “Urban” model, was conceived as an improvement over the treatment of multiple scattering in GEANT 3 [6], which was based on Molière [7] theory. It belongs to the category of condensed simulation algorithms, which account for the global effects of a large number of collisions over a track segment, including the change of direction, net displacement and energy loss of a charged particle. Geant4 “Urban” model is based on Lewis [8] theory; details about its theoretical approach and its original implementation in Geant4 can be found in [9].

A quantitative experimental validation of an early implementation of the “Urban” algorithm, concerning high energy muons, is documented in [10]: it demonstrates that the algorithm implemented in Geant4 0.1, with further improvements released in Geant4 1.0, provided better simulation accuracy than the GEANT 3.15 algorithm.

Geant4 simulation of multiple scattering based on Lewis theory has evolved since then. Various “Urban” models have been implemented; the latest Geant4 version (9.5p01) at the time of writing this paper includes four variants of this model, implemented in the *G4UrbanMscModel90*, *G4UrbanMscModel92*, *G4UrbanMscModel93* and *G4UrbanMscModel95* classes. Modifications to the original algorithm and results of their application are documented in a dedicated report [11] and in a series of conference papers [12]-[21].

The evolution of the “Urban” multiple scattering models has affected the longitudinal pattern of energy deposition: reference [1] documents the simulation accuracy achieved using the electron multiple scattering algorithm in Geant4 8.1p02 and 9.1 versions, while reference [2] highlights significant differences in the energy deposited in water by protons of approximately 70 MeV energy over several Geant4 versions from 8.1 to 9.3. In both these references other Geant4 physics models contributing to determine the energy deposition patterns were verified not to have changed over the Geant4 versions subject to test, or their evolutions resulted in statistically insignificant effects; therefore, the observed differences across different Geant4 versions are likely related to evolutions in the implementation of multiple scattering.

Additional multiple scattering models have been introduced in later versions of Geant4 besides the “Urban” model: a variant [22] of the Goudsmit-Saunderson [23] model, which according to [18] is intended to provide higher accuracy for electrons and positrons, and the “Wentzel-VI” model, that [18] characterizes as designed for precise simulation of muons and hadrons.

3. Validation method

A simultaneous validation is performed to evaluate the accuracy of backscattering and energy deposition in the same experimental set-up: accurate rendering of both observables through the same physics settings is a known issue in Monte Carlo simulation, and a sensitive test of the capabilities of multiple scattering algorithms.

The validation test exploits two sets of high precision experimental data, taken by the same experimental group at Sandia laboratories. The data reported in [24] concern the longitudinal energy deposition pattern in various materials originating from a beam of electrons with energy ranging from 0.058 MeV to 1.033 MeV. The measurements involved beryllium, carbon, aluminium, iron, copper, molybdenum, tantalum and uranium as targets. The same experimental set-up was exploited to estimate the fraction of backscattered energy of the electron beam, reported in [25]: this quantity was derived from the direct measurement of the total energy deposited in the target, corrected by the calculated energy escaped from the target volume as Bremsstrahlung photons. The experimental configuration for backscattering studies involved

beryllium, carbon, titanium, molybdenum, tantalum and uranium targets. Further details about the experimental set-up and the characteristics of the measurements can be found in [24] and [25].

The simulation configuration reproduced the experimental settings; it is described in detail in [1]. The energy deposited in the sensitive layers of the target was scored to determine the energy deposition profile as a function of the electron penetration depth. The backscattering fraction BSF was estimated as described in [25]:

$$BSF = 1 - \frac{(D + E_\gamma)}{E_0}, \quad (1)$$

where D is the total energy deposited in the detector, E_γ is the energy escaping from the detector in the form of Bremsstrahlung photons and E_0 is the kinetic energy of the incident electrons.

The simulation was configured with a variety of options of electron and photon interactions available in Geant4: “Standard” (identified as *std* in the figures), based on the evaluated data libraries distributed by the Lawrence Livermore National Laboratory (identified as *liv* and “Penelope-like” (identified as *pen*). The comparison of the results deriving from the various physics configurations with the experimental data allows the evaluation of the relative accuracy of Geant4 electromagnetic modeling options.

Simulated data were produced with Geant4 8.1.p02, 9.1.p03, 9.2.p04, 9.3.p02, 9.4.p03 and 9.5 versions. The longitudinal energy deposition profiles produced by the simulation models in the low energy electromagnetic package and the multiple scattering implementation of Geant4 versions 8.1.p02 and 9.1 were analyzed in [1] with respect to the experimental data of [24]. The study in progress extends the analysis to the following Geant4 versions, also involving the models in Geant4 standard electromagnetic package and new multiple scattering models developed since the publication of [1]; moreover, it complements the validation of the energy deposition profiles with the analysis of the backscattering fraction.

The accuracy of the simulation is quantitatively estimated by means of a statistical analysis articulated over two stages: the first one consists of goodness-of-fit tests to evaluate the compatibility of the simulation results with experimental data in each test case (experimental configuration, Geant4 physics configuration and version); the second one consists of a categorical analysis, exploiting contingency tables, to quantify whether the accuracy of different physics modeling options, or of the same modeling option in different Geant4 versions, exhibit statistically significant differences. The analysis method is described extensively in [1].

4. A sample of results

The conference poster had room only for a limited sample of representative results; this paper summarizes the preliminary overview of the recent evolution and current status of Geant4 that could be presented at the conference. The complete set of results, also including the quantitative outcome of the statistical analysis, is meant to be published in a regular peer reviewed journal.

Figure 1 shows the absorbed energy profile of 1 MeV electrons in carbon, produced by different Geant4 versions. All the simulations results were produced using the default “Urban” multiple scattering model for the corresponding Geant4 version. The experimental data and the result of the simulation based on Geant4 9.1 documented in [1] are reported in all the plots. Significant discrepancies between simulation and measurements are visible in the plots concerning Geant4 9.3 and 9.4 versions.

Figure 2 shows the absorbed energy profile of 521 keV electrons in aluminium produced with Geant4 9.3.p02 and 9.5 versions, activating the default “Urban” multiple scattering model and electromagnetic models of the standard package; the simulated profiles are compared to experimental data. The plot also shows the profile resulting from the electromagnetic processes based on the Livermore evaluated data libraries and the “Urban” multiple scattering model

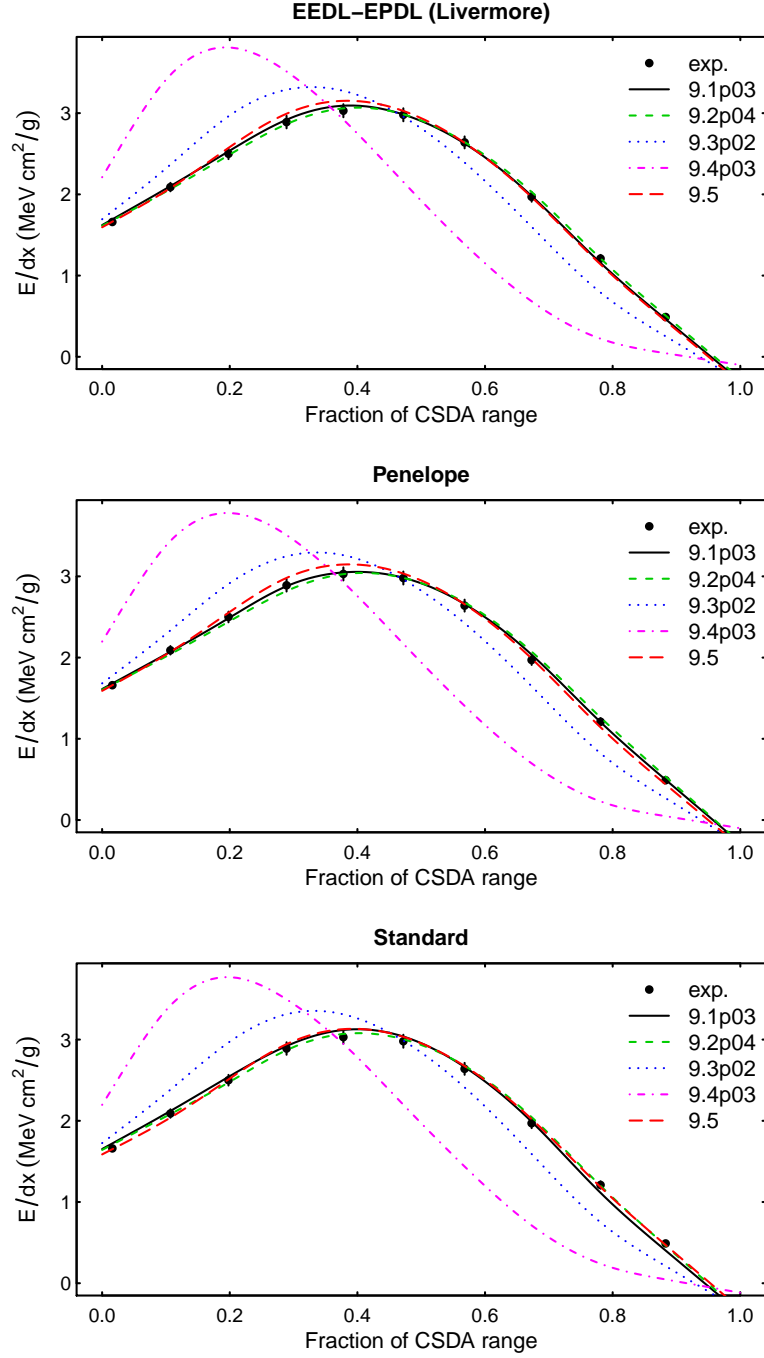


Figure 1. Longitudinal profile of energy deposition in carbon for 1 MeV electrons and different Geant4 versions, compared to experimental data. The results produced by various Geant4 modeling options are shown: “Standard”, based on the EEDL-EPDL evaluated data libraries distributed by the Lawrence Livermore National Laboratory and “Penelope-like”. The results of version 8.1 and 9.1, subject to validation in a previous work [1], are included in the plots to highlight the evolution in Geant4.

as in Geant4 9.1p03 version. The p-value from the χ^2 test of compatibility with experiment is $1.1 \cdot 10^{-90}$ for the profile produced by Geant4 9.3p02 and 0.0009 for the profile generated by Geant4 9.5. The simulation produced with Geant4 9.1p03 version is compatible with experiment with 0.01 significance.

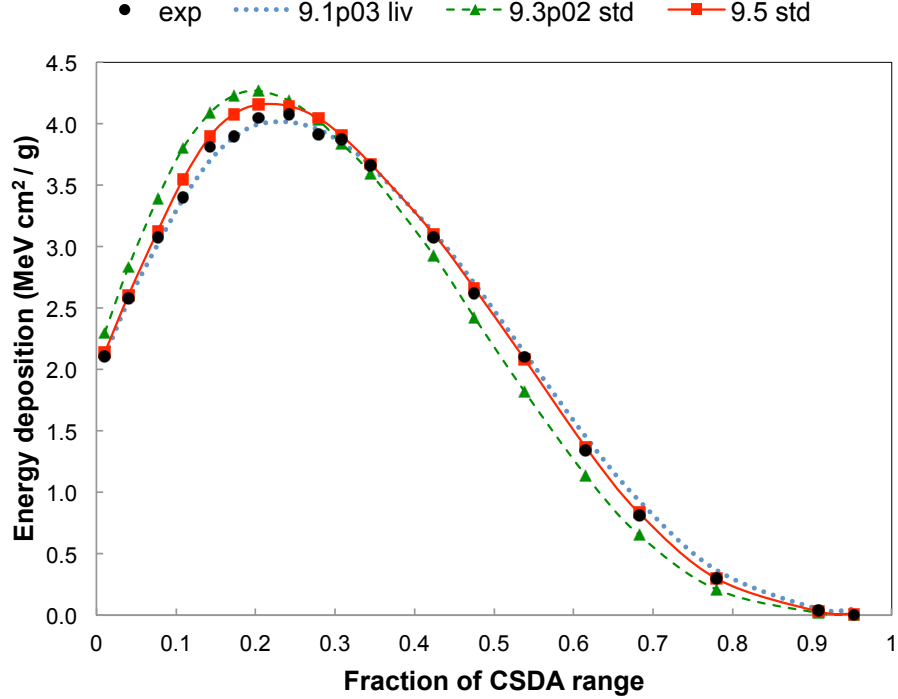


Figure 2. Energy deposition of 0.521 MeV electrons in Al: simulation with Geant4 default “Urban” multiple scattering algorithm in Geant4 9.5 (red squares) and Geant4 9.2p03 (green triangles), and experimental data (black circles) [24]. The simulation of electron-photon interactions is based on the models in the standard electromagnetic package (identified as “std”) of Geant4 9.2p03 and 9.5. The blue dotted curve represents the energy deposition profile resulting from the electromagnetic processes based on the Livermore evaluated data libraries (identified as “liv”) and the “Urban” multiple scattering model as in Geant4 9.1p03 version.

Figure 3 highlights the evolution of the energy deposition resulting from simulations where multiple scattering is modeled according to the Goudsmit-Saunderson algorithm described in [22]. The plot shows the energy deposition profiles produced by Geant4 9.3p02 and 9.5, along with experimental data. The same test case is illustrated in Figure 5 of reference [22], whose publication predates the release of Geant4 9.3. The simulation results in Figure 3 appear qualitatively different from those shown in the article documenting the original implementation of the Goudsmit-Saunderson multiple scattering model [22]. The p-value from the χ^2 test of compatibility with experiment is $1.6 \cdot 10^{-34}$ for the profile produced by Geant4 9.3p02 and $1.8 \cdot 10^{-22}$ for the profile generated by Geant4 9.5.

Table 1 reports preliminary results of the backscattering fraction, estimated according to equation 1, for a few target materials and electron beam energies; the simulation was produced with Geant4 9.3p02 version. Large differences are visible with respect to the results of [25]; the origin of these discrepancies is under investigation.

The “efficiency” of a Geant4 electromagnetic physics model is defined as the fraction of test cases in which the χ^2 test does not reject the null hypothesis of compatibility between the energy

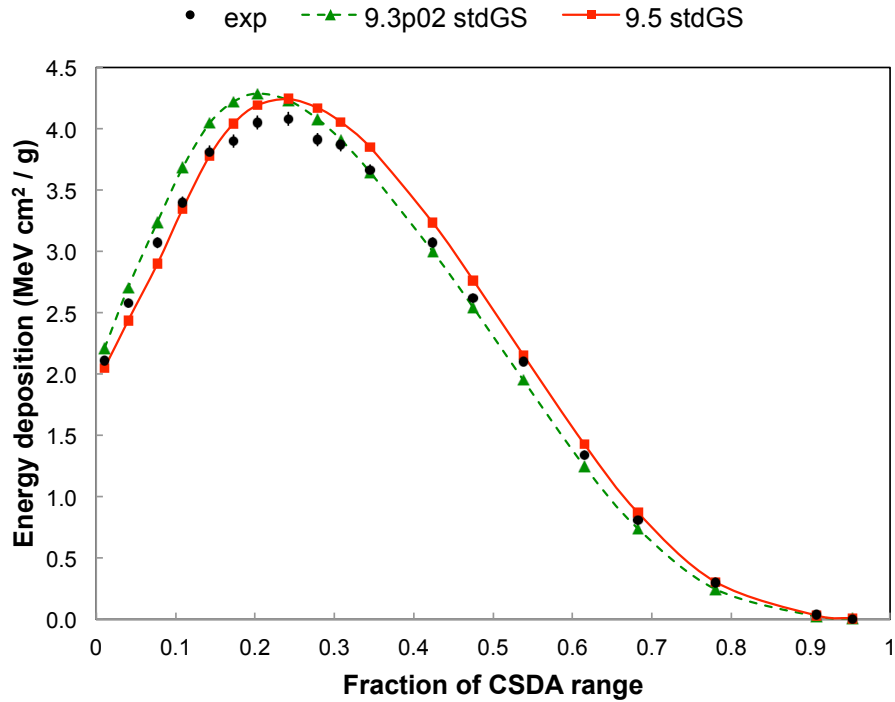


Figure 3. Energy deposition of 0.521 MeV electrons in Al, resulting from simulations with the Goudsmit-Saunderson multiple scattering algorithm in Geant4 9.5 (red squares) and Geant4 9.3p02 (green triangles), and experimental data (black circles) [24]. Electron-photon interactions are simulated with Geant4 standard electromagnetic models (identified as “std” in the plot).

Table 1. Backscattering fraction.

Material	Beam Energy	BSF Experiment	BSF Geant4 9.3p02
Tantalum	1 MeV	0.191	0.310
Carbon	1 MeV	0.028	0.020
Carbon	25 keV	0.103	0.296

deposition profile simulated by that model and experimental measurements, at 0.01 level of significance: it quantifies the capability of that simulation model to produce results statistically consistent with experiment over the whole experimental data sample of [24] involved in the validation process.

The efficiency at reproducing the measured longitudinal energy deposition profiles of [24] is summarized in Table 2 for Geant4 9.5p01, which is the latest Geant4 stable version at the time of submitting this paper to CHEP 2012 proceedings, and for the Geant4 version validated in [1]. The efficiencies reported in the table correspond to the three Geant4 electromagnetic models (“Livermore”, “Penelope-like” and “Standard”) associated with default electron multiple scattering settings in the respective Geant4 version. This table provides guidance to Geant4 users on which electromagnetic model to use in the latest version of Geant4 to achieve higher accuracy, and shows how the simulation accuracy achievable in the latest version has evolved with respect to the performance in a previously validated Geant4 version.

Table 2. Efficiency of Geant4 models at reproducing experimental energy deposition profiles.

Model	Geant4 9.5p01	Geant4 9.1p03
Livermore	0.47 ± 0.09	0.73 ± 0.08
Penelope	0.13 ± 0.06	0.30 ± 0.08
Standard	0.17 ± 0.07	0.17 ± 0.07

Conclusions

The preliminary results summarized here show that different versions of Geant4 produce visibly different energy deposition profiles resulting from the interaction of electrons with energy up to 1 MeV, when the same conditions (geometry, beam energy, target material, nominal physics configuration) are compared. Statistical analysis based on goodness-of-fit tests confirms that the energy deposition distributions produced by some Geant4 versions exhibit a significant disagreement with respect to experimental data. Incompatibility with the experimental reference is also evident in a preliminary analysis of the backscattering fraction calculated by one of such versions.

The similar behaviour exhibited by different Geant4 electromagnetic models in the context of the same Geant4 version suggests that energy deposition patterns are strongly affected by the evolution of the implementation of the *Urban* multiple scattering model, which is common to the simulations activating different electron-photon interaction models.

Variations in the energy deposition patterns are visible when different multiple scattering models are activated (e.g. *Urban* and *Goudsmit-Saunderson*). This observation suggests that factors other than multiple scattering algorithms also contribute to the observed different behaviour with respect to experimental measurements resulting from different Geant4 versions.

Further work is in progress to complete the statistical data analysis, that quantifies the evolution and current status of Geant4 simulation accuracy at reproducing the experimental data of [24] and [25]. The results will be documented in a forthcoming publication.

Acknowledgments

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